

nlFIT - Nonlinear Fitting by Gauss-Newton

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This program allows nonlinear fitting by the Gauss-Newton method for an equation entered by the user. The program was adapted from the DATFIT program code (Coffin, 1995). It has the logistics and differentials given below.

1 Files

1. *nlFIT* - program file
2. *exNLF* - example file

2 Program structure

1. Direct data entry into the stack as lists, without the need for a form (INFORM);
2. Number of iterations requested in the initial input;
3. There is only one data input, not two as in the original code;
4. The index for each iteration is displayed in the upper left corner of the graphical screen;
5. Provides as output:
 - a. covariance matrix;
 - b. calculated parameter values;

- c. standard deviation values of the parameters;
 - d. regression chi-square;
 - e. list of xi values;
 - f. list of y_calc values
 - g. graphic screen with experimental points;
 - f. nonlinear fit curve superimposed on the points;
6. Uses the FDER and PGALL subroutines from the same book to calculate the symbolic derivative of the equation and to eliminate previously stored variables, *respectively* (the original program requires 3 subprograms to run);
 7. Plot the experimental data with a routine that does not use Σ DAT (PIXON).

3 Data entry

To use the program, the following data must be entered in the stack sequence:

- ```
Data entry
```
1. list of xi values: {x1 x2...xn};
  2. list of yi values: {y1 y2 y3, ...yn};
  3. list of weights: {w1, w2, w3, ...wn}. Note: if there are no weights, enter a unit list - {1 1 1...};
  4. adjustment *equation* (e.g.,  $V_m \cdot x / (K_m + x)$ ; equation for Michelis-Mentem enzyme kinetics).  
Note: independent variable as "x";
  5. list of parameters seeds: {p1 p2}. Note: in the example, p1 =  $V_m$  and p2 =  $K_m$ ;
  6. number of desired iterations. Ex: 3

### 4 Program use

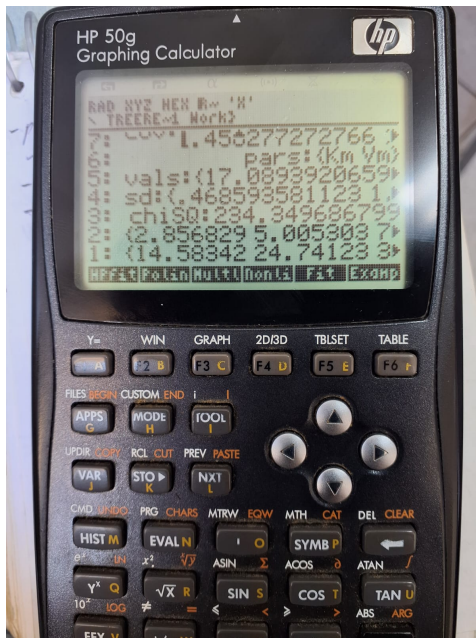
Attached to the compressed file is an example in enzyme kinetics to illustrate its use:

# Using the program

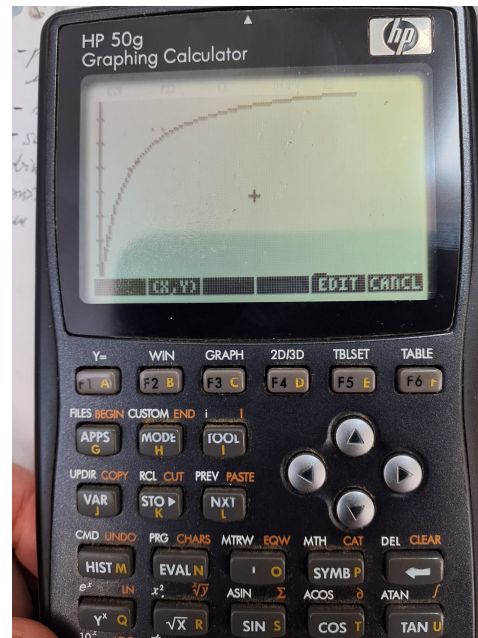
1. Click on EVAL in the example file to release the necessary input lists;
2. Click on "nlFIT" to run the program;

NOTE: For user data, simply replace the lists.

## 5 Results



(a) Results



(b) Scatter plot and nonlinear fit

Figure 1: HP50G screens showing the text and graph results of *nlFIT*.

## Author

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## Reference

Coffin, Dan. Calculus on the HP 48G/GX. Grapevine Publications, 1995.